2-Nitrobenzamide

610-15-1 | DTXSID0025733

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 42.6 L/kg

Global applicability domain: Inside

Local applicability domain index: 6.04e-01

Confidence level: 8.14e-01

Nearest Neighbors from the Training Set

Image not found
2-Nitrobenzamide
Measured: 28.2
Predicted: 42.6

Image not found
3-Nitrobenzamide
Measured: 89.1
Predicted: 64.5

Image not found
2-Chlorobenzamide
Measured: 32.4
Predicted: 37.2

Image not found
4-Nitrobenzamide
Measured: 85.1
Predicted: 68.2

Image not found
Benzamide, 4-methyl-
Measured: 60.3
Predicted: 48.4